1,3-DIBROMO-5-FLUOROBENZENE

Inchi: InChI=1S/C6H3Br2F/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey: ASWYHZXKFSLNLN-UHFFFAOYSA-N
Formula: C6H3Br2F
SMILES: Fc1cc(Br)cc(Br)c1
Mol. weight [g/mol]: 253.90

Physical Properties

Property code	Value	Unit	Source
hfus	18.21	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.351		Crippen Method
mcvol	108.410	ml/mol	McGowan Method
tb	472.80	K	Cheméo Relay (1.0)
tf	307.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.55	J/mol×K	504.91	Joback Method
cpg	178.77	J/mol×K	545.53	Joback Method
cpg	185.41	J/mol×K	586.15	Joback Method
cpg	191.50	J/mol×K	626.77	Joback Method
cpg	197.08	J/mol×K	667.39	Joback Method
cpg	202.20	J/mol×K	708.00	Joback Method
cpg	206.91	J/mol×K	748.62	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435514&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point